

Towards Predicting Thermal Runaway of Lithium-Ion Batteries

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Motivation and Goal

The thermal runaway of lithium-ion batteries poses a severe safety threat for large-scale lithium-ion battery applications. This cooperation project aims in developing a profound understanding of the electro-chemical mechanisms that trigger thermal runaway and to predict its probability via stochastic methods. The general methodology and preliminary numerical results are presented.

Multi-Scale Deterministic Model

1. Transport

Three transport processes at three different scales are considered. Heat transport is solved with COMSOL; charge and ion transport are solved in in-house software DENIS [1]

i.) Heat transport (mm scale, 3D, COMSOL)

$$\frac{\partial(\rho c_p T)}{\partial t} = \nabla \cdot (k \nabla T) + \dot{Q}_{\text{elchem}} + \dot{Q}_{\text{ohm}}$$

ii.) Charge transport in electrolyte (μm scale, 1D, DENIS)

$$\frac{\partial(\epsilon c_i)}{\partial t} = \frac{\partial}{\partial y} \left(D_i(c_i, T) \frac{\partial c_i}{\partial y} \right) + \frac{z_i F}{RT} \frac{\partial}{\partial y} \left(D_i(c_i, T) c_i \frac{\partial \phi}{\partial y} \right) + M_i \dot{s}_i^V$$

iii.) Lithium diffusion (nm scale, 1D, DENIS)

$$\frac{\partial \rho_{\text{Li}}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 D \frac{\partial \rho_{\text{Li}}}{\partial r} \right) - \frac{M_{\text{Li}}}{zF} i$$

2. Kinetics

Butler-Volmer equation

$$i = i_0 \left(\exp \left(\frac{\alpha F}{RT} (\eta_{\text{act}} - R_{\text{SEI}} \cdot i) \right) - \exp \left(-\frac{(1-\alpha)F}{RT} (\eta_{\text{act}} - R_{\text{SEI}} \cdot i) \right) \right)$$

Overpotentials

Concentration

$$\eta_{\text{conc}} = \frac{RT}{zF} \ln \left(\frac{c_0}{c(t)} \right)$$

Activation

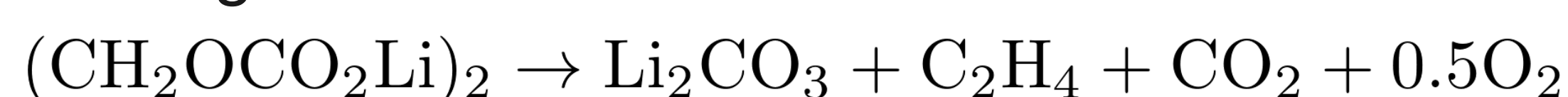
$$\eta_{\text{act}} = \Delta \phi(t) - \Delta \phi_{\text{eq}}(c_{\text{Li}}) - \eta_{\text{conc}}$$

3. Thermal decomposition model

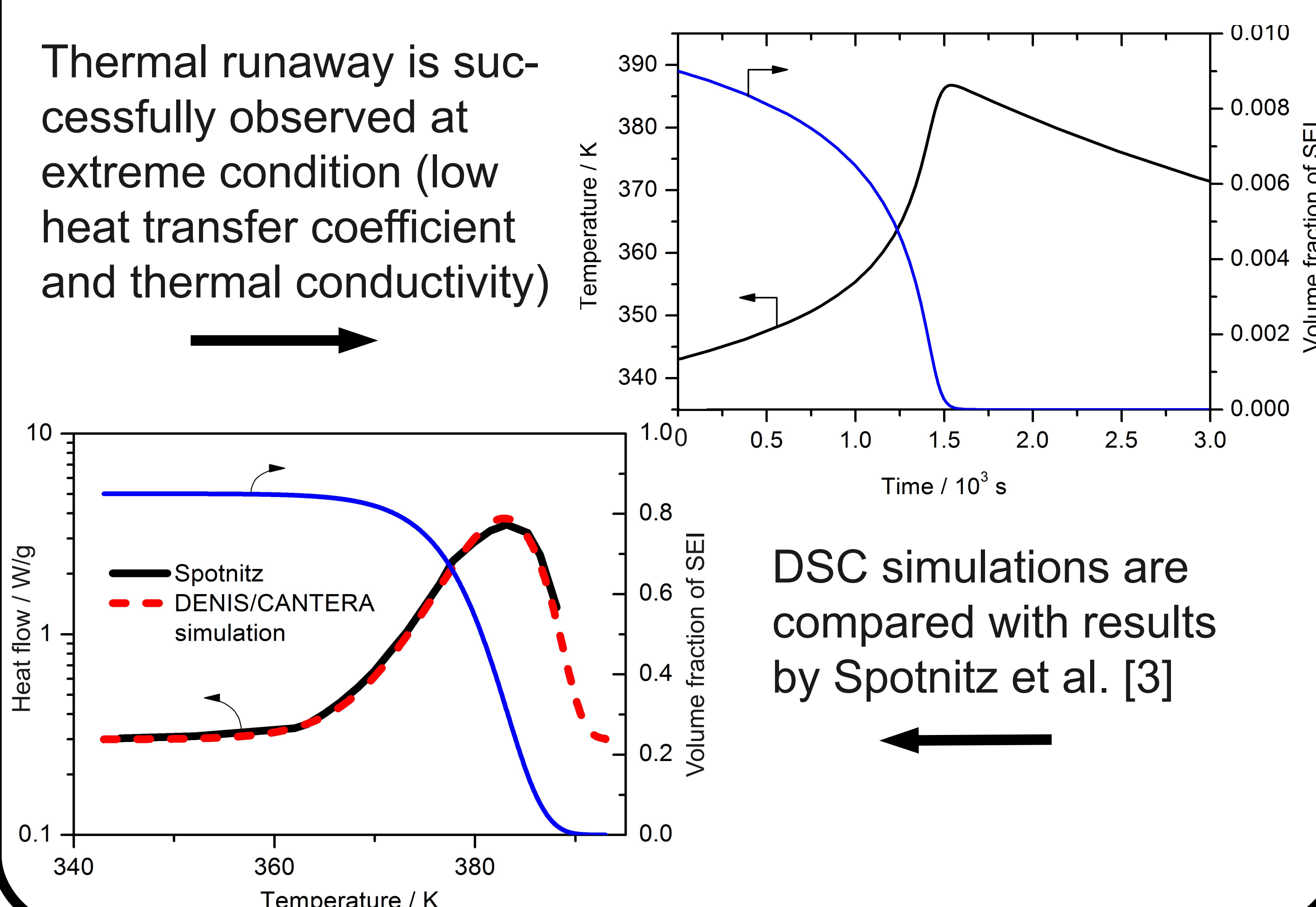
The model is coupled to CANTERA [2]. This will allow to model several decomposition reactions.

Model results

As a preliminary study, a solid electrolyte interface decomposition is investigated:



Thermal runaway is successfully observed at extreme condition (low heat transfer coefficient and thermal conductivity)



Experimental Analysis

Data from own experiments will allow to conduct plausibility checks for the models. Planned experiments include:

- performance experiments
- abuse experiments (external heating, nail penetration, overcharge, external short-circuit)

Available calibration data will thus comprise cell surface and ambient temperatures, current and voltage

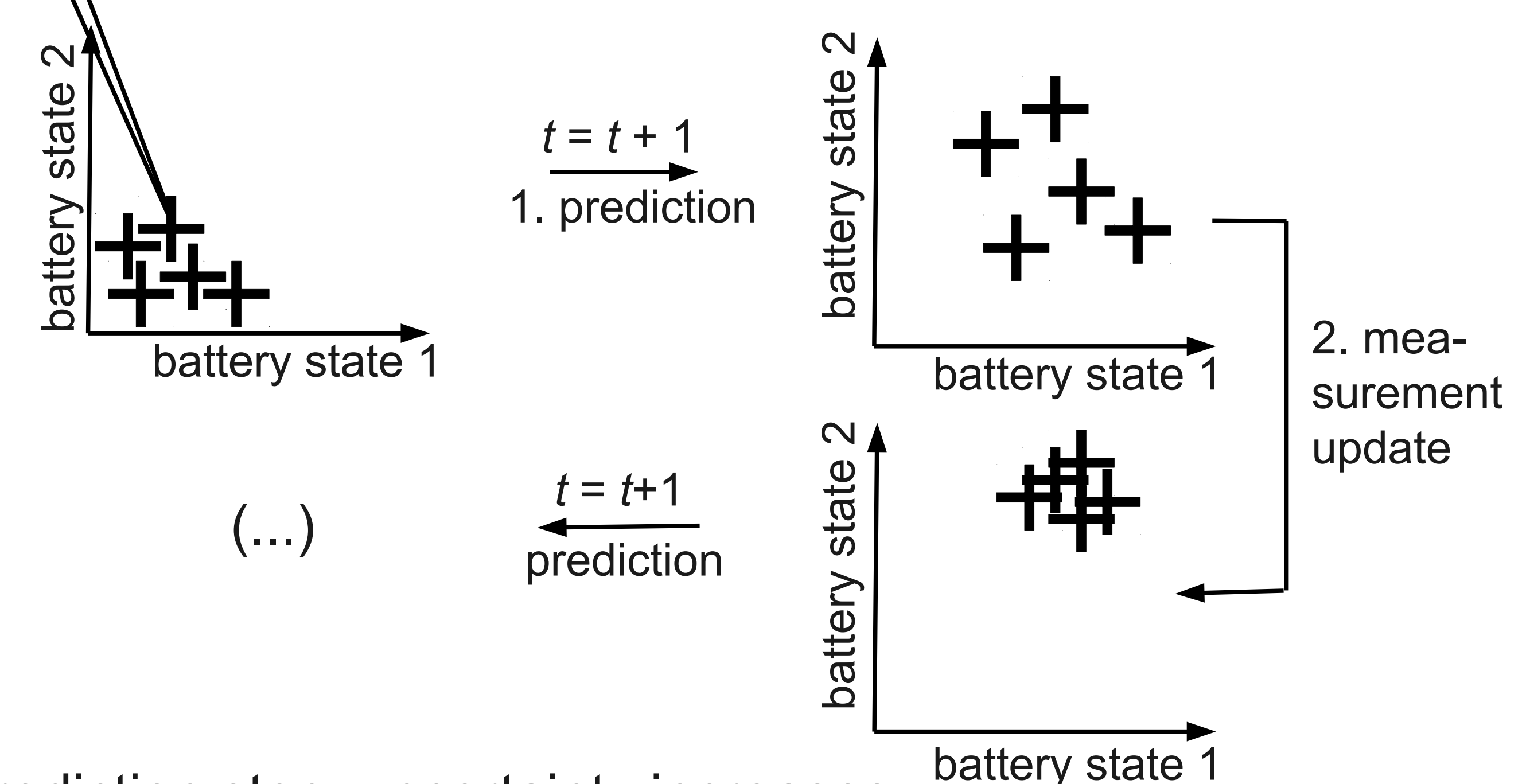
Stochastic Simulation

Sources of uncertainty: model errors, parameter errors, measurement errors etc.

⇒ From runaway (yes/no) to probabilities (0%, ..., 100%)

How likely will battery undergo thermal runaway in near future?

Monte-Carlo simulations and particle filters:



Prediction step: uncertainty increases
Update step: uncertainty decreases

Goals of Simulation

- Identification of critical areas in state space
- Real-time simulation of runaway risk
- Real-time updating to sensor data
- Control scheme for risk minimization

References

- [1] W. G. Bessler, S. Gewies and M. Vogler, *Electrochimica Acta* 53 (2007) 1782 – 1800
- [2] D. G. Goodwin, <http://code.google.com/p/cantera> (2001-2010)
- [3] R. Spotnitz and J. Franklin, *Journal of Power Sources* 113 (2003) 81-100

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